Converting NO_2 to NO_x emissions from NO_2 satellite observations

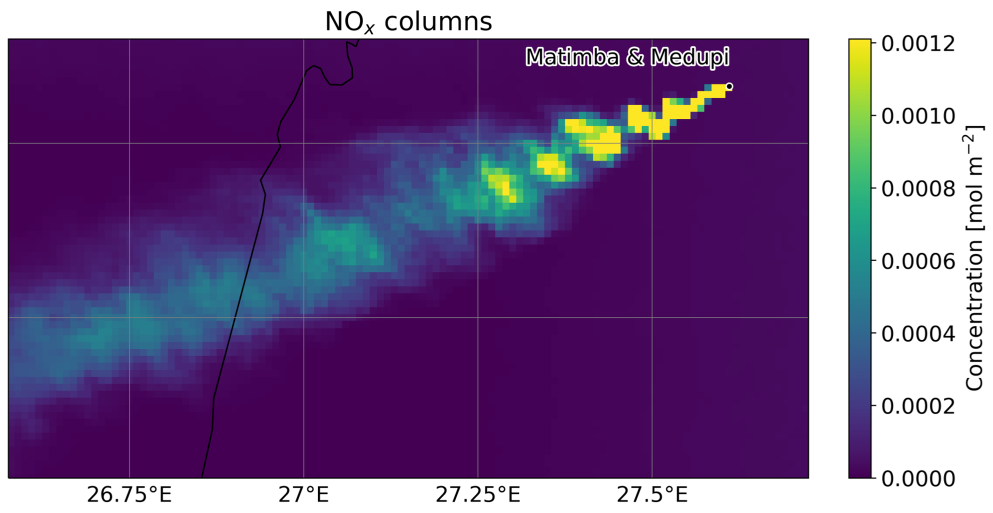
Sandro Meier[1,2], Erik F. M. Koene[1], Maarten Krol[3,4], Dominik Brunner[1], Alexander Damm[2,5], and Gerrit Kuhlmann[1]
[1]Empa, Laboratory for Air Pollution / Environmental Technology, Switzerland
[2]Department of Geography, University of Zurich, Switzerland
[3]Meteorology and Air Quality, Wageningen University & Research, The Netherlands
[4]Institute for Marine and Atmospheric Research Utrecht (IMAU), Utrecht University, The Netherlands
[5]Eawag, Swiss Federal Institute of Aquatic Science & Technology, Surface Waters – Research and Management, Switzerland

1. Introduction

- **Nitrogen oxides** (NO_x = NO + NO_2) are important air pollutants which are emitted during high-temperature combustion processes.
- Monitoring NO_x emissions is crucial for assessing **air quality** and for providing **proxy estimates of CO_2 emissions**.
- Satellite observations, e.g., from the TROPOspheric Monitoring Instrument (**TROPOMI**), provide **global coverage at high temporal resolution**. While most NO_x is emitted as NO, satellites only measure NO_2, necessitating a **conversion to NO_x**.
- Previous studies often applied a constant NO_2-to-NO_x conversion factor of about 1.3, derived assuming steady-state conditions [1].
- We developed a more **realistic model for NO_2 to NO_x conversion** and applied it to TROPOMI data of 2020 and 2021 [2].

2. Simulation of realistic NO_x plumes

Plume-resolving simulations using **MicroHH** Large Eddy Simulations **with chemistry** for the power plants Bełchatów (PL), Jänschwalde (DE), Matimba and Medupi (ZA), and a metallurgical plant in Lipetsk (RU) [3].



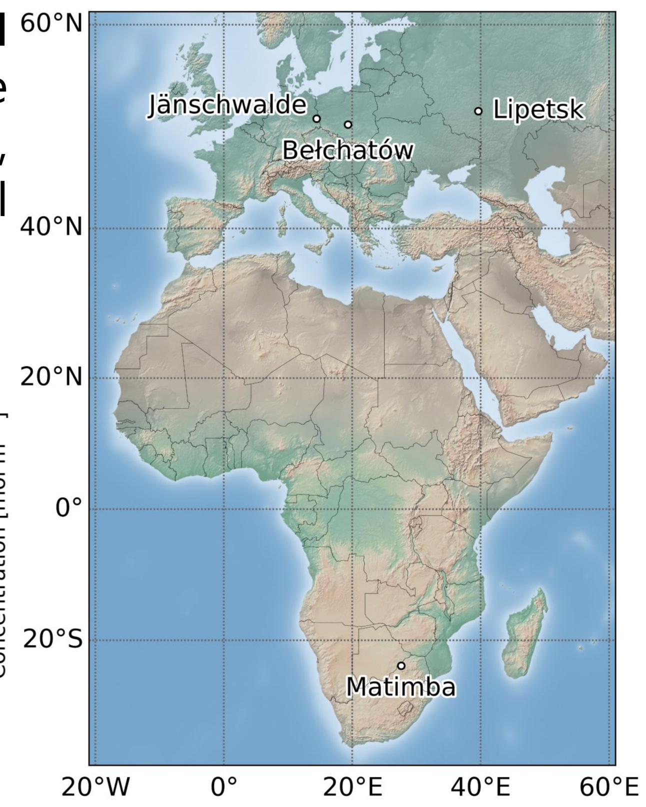
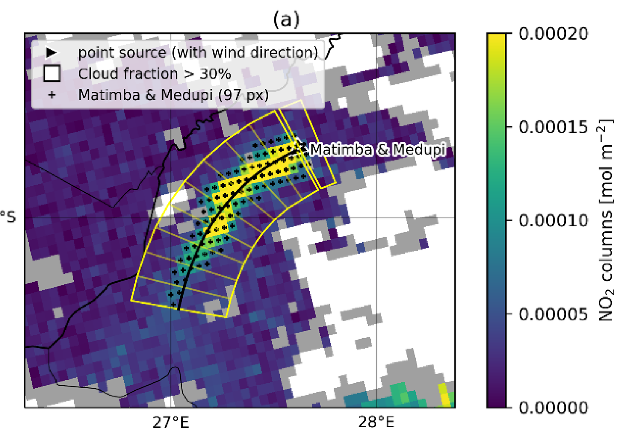


Figure 1: Left: Example of simulated NO_2 and NO_x columns from the MicroHH simulation of Matimba & Medupi at a resolution of 100 × 100 × 50 m. Right: Location of the simulated sources.

3. Cross-sectional flux method



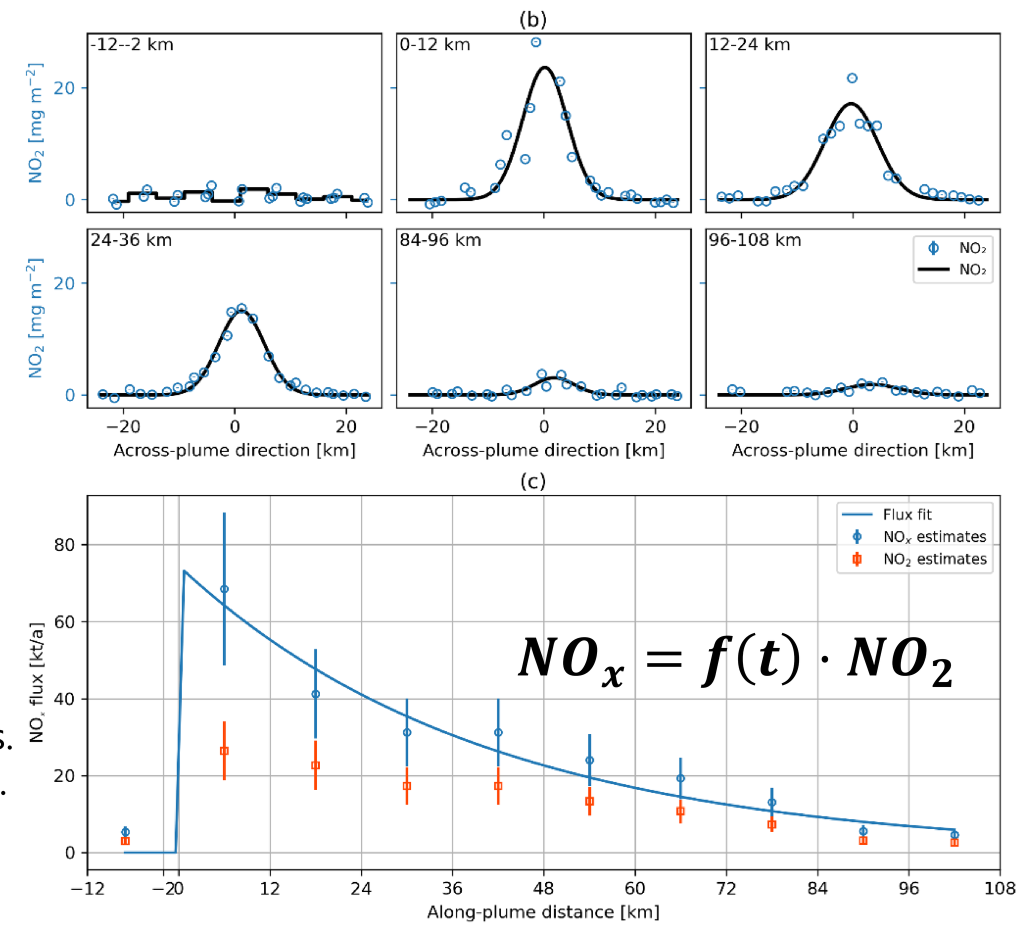


Figure 2: Example of the cross-sectional flux method used to estimate NO_x emissions.
(a) Satellite image of a NO_2 plume divided into sub-polygons.
(b) NO_2 cross sections for six sub-polygons with fitted line densities.
(c) Along plume NO_2 and NO_x fluxes.
(d) Estimated emissions and decay time are 75 kt/a and 3.2 hours.

4. NO_2-to-NO_x conversion factors

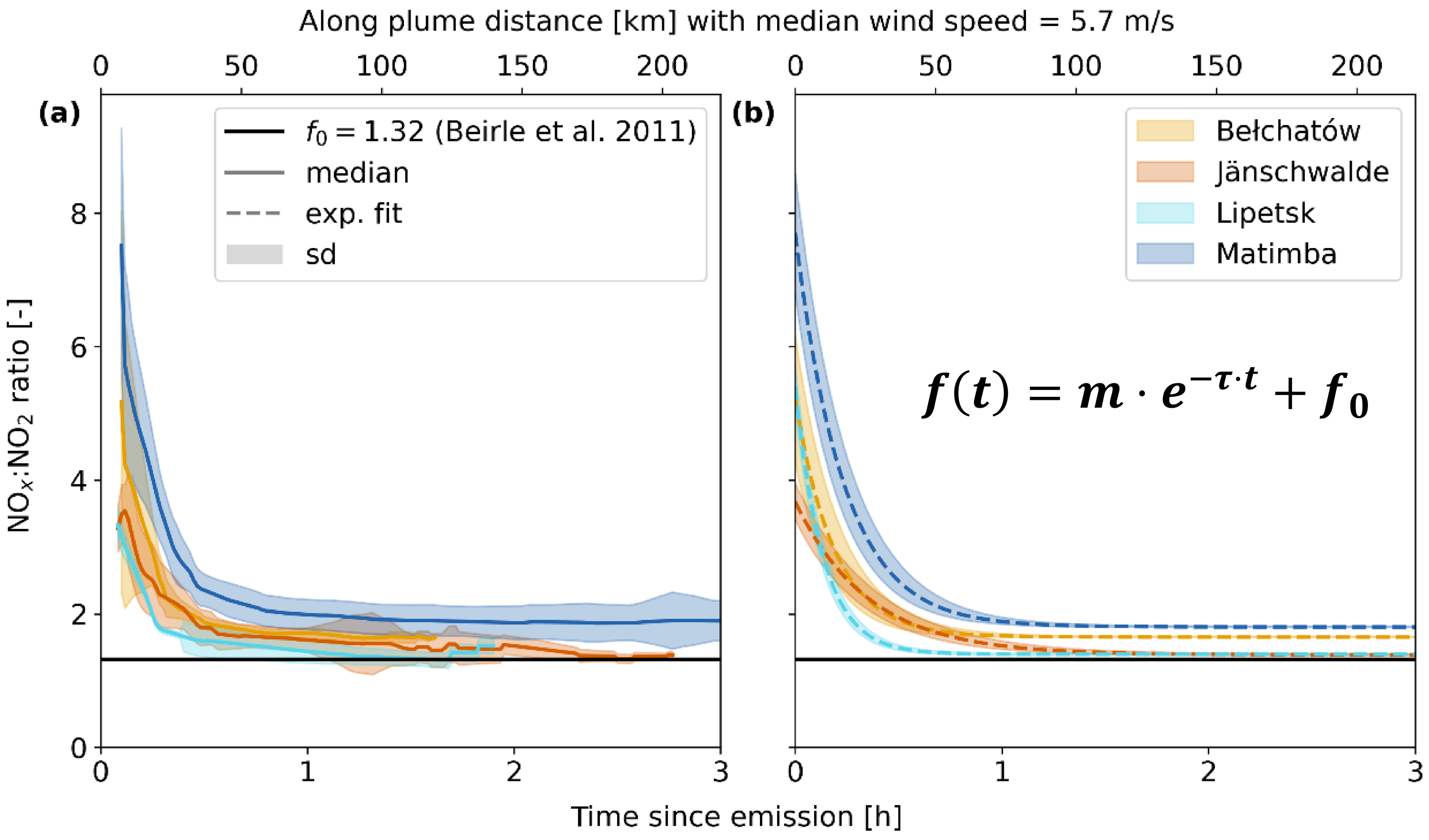


Figure 3: NO_x:NO_2 ratios of the MicroHH time steps 8-14 UTC. The time since emission is computed from an effective wind speed at the source and the plume length.

5. Validation with MicroHH data

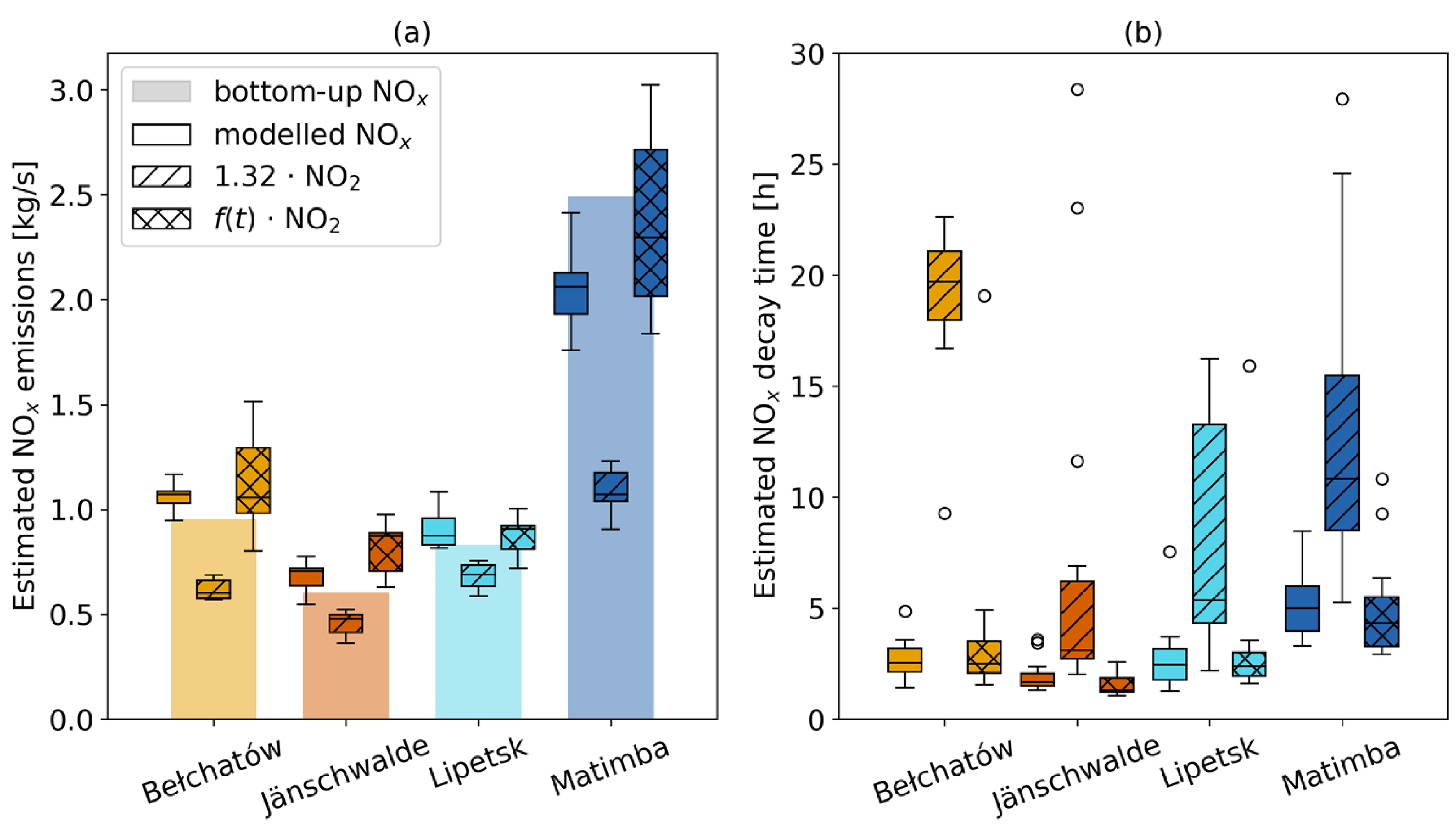


Figure 4: Comparison of estimated NO_x emissions (a) and decay times (b) using the constant and time-dependent algorithms as well as the modelled NO_x fields.

6. Application to TROPOMI NO_2 data

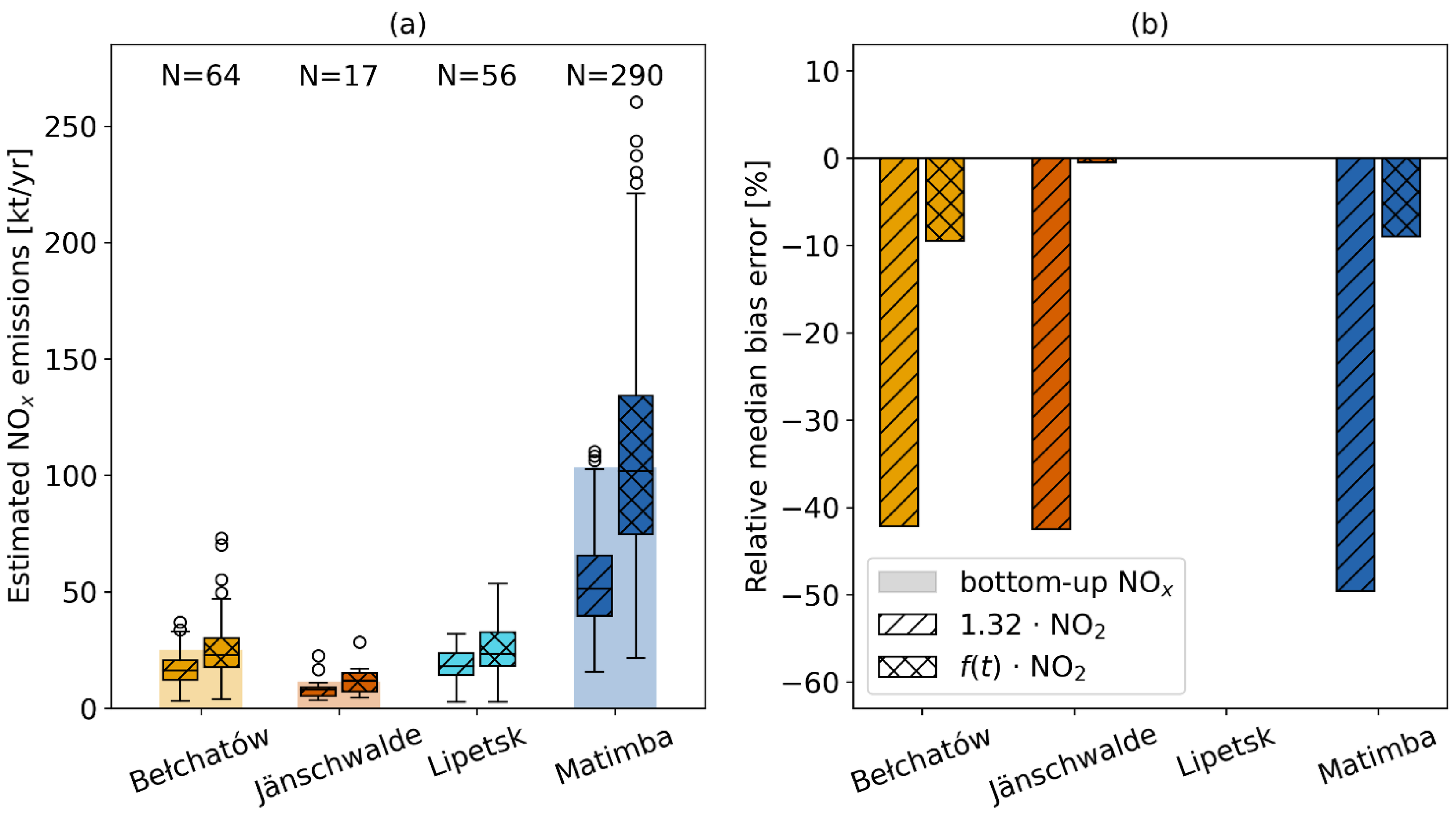


Figure 5: Estimated NO_x emissions and their biases for TROPOMI data of the years 2020 and 2021.

7. Key findings & Conclusion

- Most of the NO_x is emitted as NO → complete titration of O_3 close to the source → high NO_x:NO_2 ratios.
- With increasing dilution and mixing of the plume → accelerated oxidation of NO to NO_2 → lower NO_x:NO_2 ratios.
- Estimated NO_x emissions using NO_2-to-NO_x conversion factors which depend on the time since emission **agree** with the estimates from the **modelled NO_x fields** in MicroHH.
- **Biases** in estimated NO_x emissions from TROPOMI NO_2 observations are **greatly reduced** when using NO_2-to-NO_x conversion factors which depend on the time since emission.
- **More simulations** covering a wider range of meteorological and trace gas background conditions are **needed to generalize the approach**.
- NO_2-to-NO_x conversion model **implemented in open-source Python library** for data-driven emission quantification (ddeq) [4]

Contact
Sandro Meier
sandro.meier@empa.ch
www.linkedin.com/in/sandro-meier98

Acknowledgements
The research was funded by the Horizon Europe CORSO project (no. 101082194) with additional funding by the Swiss State Secretary for Education, Research and Innovation (SERI, no: 22.00422).

References
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